Carbazole-2-carbonitrile, 5,6,7,8-tetrahydro-1-methyl-
73771-63-8 | DTXSID50224153

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.81e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.46e-01

Confidence level: 1.94e-01

Nearest Neighbors from the Training Set

Image not found
2,3-Benzofluorene
Measured: 1.35e-04
Predicted: 2.22e-07

Image not found
Triphenylene
Measured: 2.08e-05
Predicted: 1.87e-08

Image not found
Methyl salicylate
Measured: 5.27e-06
Predicted: 4.27e-03

Image not found
Clofentezine
Measured: 5.33e-11
Predicted: 1.59e-09